

Exceptional service in the national interest

ME469: Numerical Abstractions

Stefan P. Domino^{1,2}

¹ Computational Thermal and Fluid Mechanics, Sandia National Laboratories

This presentation has been authored by an employee of National Technology & Engineering Solutions of Sandia, LLC under Contract No. DE-NA0003525 with the U.S. Department of Energy (DOE). The employee owns all right, title and interest in and to the presentation and is solely responsible for its contents. The United States Government retains and the publisher, by accepting the article for publication, acknowledges that the United States Government retains a non-exclusive, paid-up, irrevocable, world-wide license to publish or reproduce the published form of this article or allow others to do so, for United States Government purposes. The DOE will provide public access to these results of federally sponsored research in accordance with the DOE Public Access Plan



²Institute for Computational and Mathematical Engineering, Stanford

Useful Abstractions

Real World

The intended application

Conceptual Model

 Physical laws, hypothesis and models (e.g. a set of PDEs) and initial and boundary conditions

Computer Model

A set of computational algorithms that allow to build a numerical, or approximated solution to the conceptual model



Mappings:

Real World

Conceptual Model

(

Computer Model



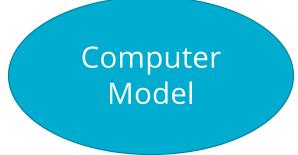
Qualification: Adequacy of the conceptual model to provide an acceptable level of agreement for the intended application

Real World

Conceptual Model

Examples:

- Is the fluid Newtonian?
- Are compressibility effects important?
- Uniform or variable-density?
- Isothermal or non-isothermal?





<u>Verification</u>: **Process of determining that (1) the model implementation faithfully represents the conceptual model (without mistakes) and (2) the solution to the model is accurate**

Real World

Examples:

- Is it RHS += A, RHS -=A? Which is correct?
- Should the contribution be scaled by a volume?
- How does the Quantity of Interest (QoI) behave as a function of mesh or time step resolution?

Conceptual Model

Verification

Computer Model



<u>Validation</u>: **Process of determining the degree to which the numerical solutions** (hence the model) is an accurate representation of reality from the perspective of the intended application

Real World

Conceptual Model

Examples:

- Midterm project: compare drag coefficient prediction to an experiment
- Final project: compare drag coefficient for flow past rotating shapes; chaotic flow prediction at a given configuration

Validation

Computer Model

Verification vs Validation (V&V)? The Formal Lexicon

Verification: Are we solving the equations correctly?

- Represents an exercise in computational mathematics
- Given an equation, is the solution converging at known rates?

<u>Validation</u>: Are we solving the correct equations?

 Represents an exercise in understanding the physics associated with the real world use case

In this course, we will strongly focus on *verification*

- Establishing the correctness of the numerical implementation is key
- Comparisons of the numerical results to reality is not the primary objective

Verification challenges?

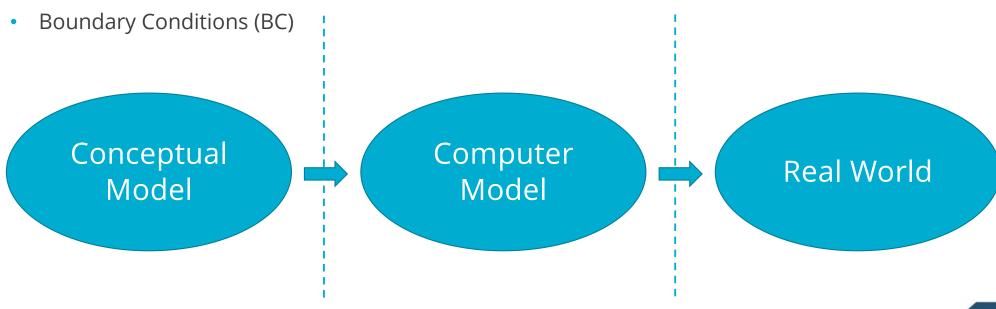
- Knowledge of the true solution, i.e., exact analytical solutions
- How many exact solutions exist for our class of physics? Not many!
- Hint: Method of Manufactured Solutions (MMS)



The Construction of a Numerical Method: Discretization and Solution

Mathematical Formulation

- Partial differential equations (PDE)
- Initial Conditions (IC)





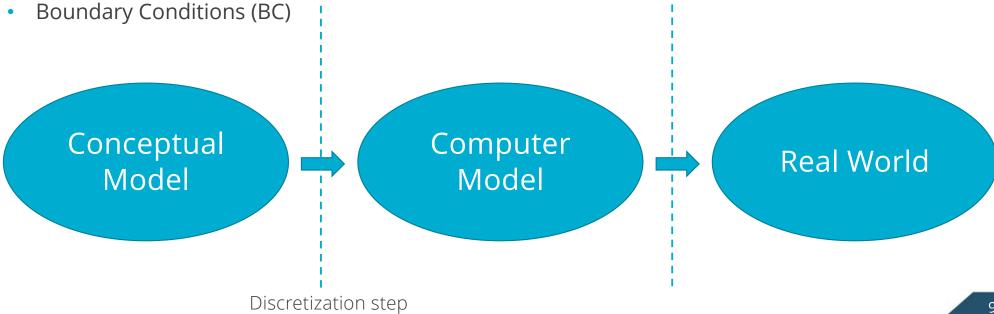
The Construction of a Numerical Method: **Discretization and Solution**

Mathematical Formulation

- Partial differential equations (PDE)
- Initial Conditions (IC)

Numerical Formulation

- Discretize in space and time
- Algebraic Differential Equations (ADE)





The Construction of a Numerical Method: Discretization and Solution

Mathematical Formulation

- Partial differential equations (PDE)
- Initial Conditions (IC)
- Boundary Conditions (BC)

Numerical Formulation

- Discretize in space and time
- Algebraic Differential Equations (ADE)

Numerical Solution

- Algebraic Differential Equations (ADE)
- Linear solvers
- Convergence, mesh adequacy,?

Conceptual Model Computer Model

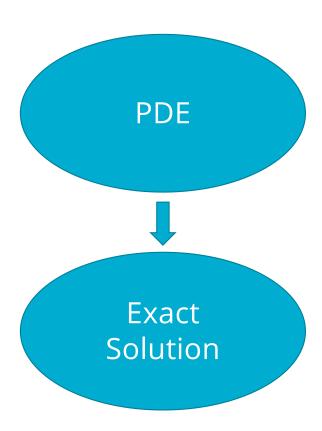
lodel

!Real World

Discretization step

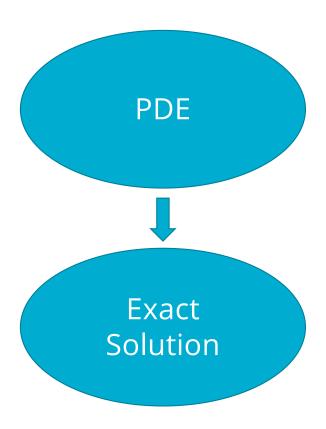
Solution step



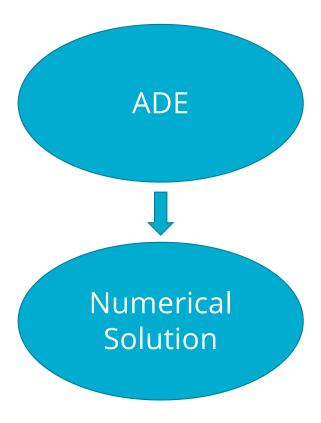


What we would like to have...



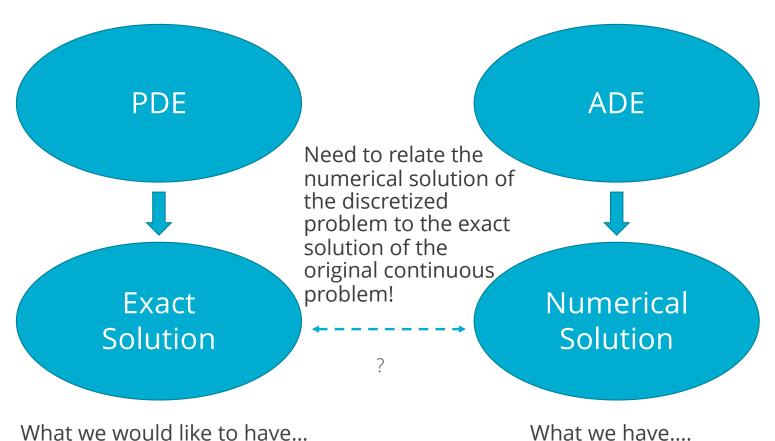


What we would like to have...

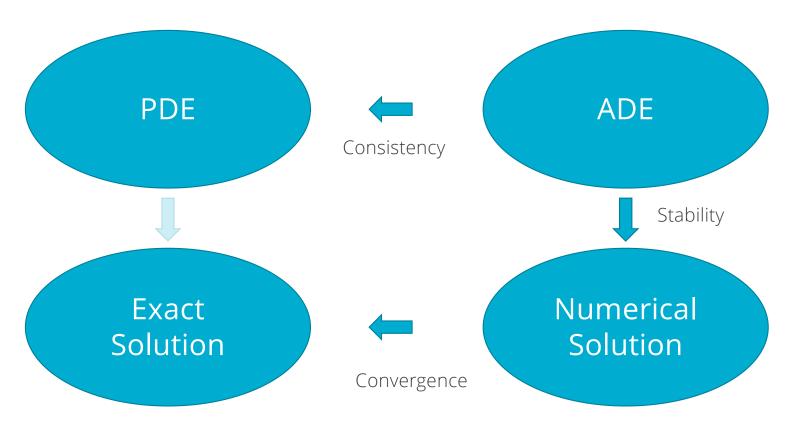


What we have....





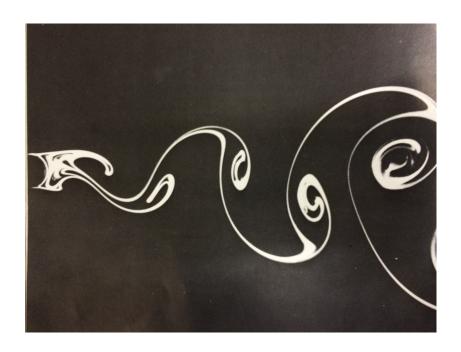




• For a well-posed, <u>linear PDE</u>, Lax-Richtmyer Equivalence Theorem, AKA the Fundamental Theorem of Numerical Analysis: Consistency + Stability = Convergence



Example 1: Vortex Street



Conceptual Model

Computer Model

Real World?



Example 2: Modeling a Luminaria – In the Snow!



Conceptual Model

Computer Model

Real World?